

A Direct Prediction of the Shape Parameter—a purely scattered data approach

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Abstract. In this paper we present an approach which predicts directly without search the optimal choice of the shape parameter c contained in the multiquadrics $(-1)^{\lceil \frac{\beta}{2} \rceil} (c^2 + \|x\|^2)^{\frac{\beta}{2}}$, $\beta > 0$, and the inverse multiquadrics $(c^2 + \|x\|^2)^{\frac{\beta}{2}}$, $\beta < 0$. Unlike the simplex scheme where the data points are required to be evenly spaced, as in a recent paper of the author, here we allow them to be arbitrarily scattered in the simplex, making it much more useful. The drawback is that its theoretical ground is not so strong as in the evenly spaced data setting. However, experiments show that it works well. The experimentally optimal value of c coincides with the theoretically predicted one. Since the fill distance involved is always of reasonable size, this approach is supposed to be practically useful.

Key words: radial basis function, multiquadric, shape parameter, interpolation

AMS: 41A05, 65D05, 65M15, 65M70, 65N15, 65N50

1 Introduction

In this paper the approximated functions lie in a space called B_σ as in the following definition.

Definition 1.1 *For any $\sigma > 0$, the class of band-limited functions f in $L^2(R^n)$ is*

$$B_\sigma := \{f \in L^2(R^n) : \hat{f}(\xi) = 0 \text{ if } |\xi| > \sigma\},$$

where \hat{f} denotes the Fourier transform of f .

This function space looks small. In fact, it plays only an intermediate role in the interpolation. Via the B_σ functions, all functions in the Sobolev space can be interpolated by the multiquadrics or inverse multiquadrics, as will be explained further in the paper.

The radial function we adopt is

$$h(x) := \Gamma(-\frac{\beta}{2})(c^2 + \|x\|^2)^{\frac{\beta}{2}}, \quad \beta \in R \setminus 2N_{\geq 0}, \quad c > 0, \quad (1)$$

where $\|x\|$ is the Euclidean norm of $x \in R^n$, Γ is the classical gamma function, and β , c are constants. Note that this definition is slightly different from the one mentioned in the abstract. The definition

(1) will simplify its Fourier transform and the presentation of our central theorem. The function $h(x)$ in (1) is conditionally positive definite (c.p.d.) of order $m = \max\{0, \lceil \frac{\beta}{2} \rceil\}$ where $\lceil \frac{\beta}{2} \rceil$ means the smallest integer greater than or equal to $\frac{\beta}{2}$. For further details we refer the reader to Madych and Nelson [1] and Wendland [2].

For any set of data points (x_j, y_j) , $j = 1, \dots, N$, where $X = \{x_1, \dots, x_N\}$ is a subset of R^n and y_j are real or complex numbers, we can always find an interpolant of the form

$$s(x) = p(x) + \sum_{j=1}^N c_j h(x - x_j), \quad (2)$$

where $p(x)$ is a polynomial in P_{m-1}^n , $m = \max\{0, \lceil \frac{\beta}{2} \rceil\}$, and c_j are coefficients to be chosen, as long as X is a determining set for P_{m-1}^n . Interested readers can find these in [1].

Although we are interested only in scattered data, our criteria of choosing c are developed from a core theorem which involves a simplex scheme with evenly spaced data points, as mentioned in the abstract. Therefore it is necessary to make a brief description of the evenly spaced scheme.

Let T_n denote an n -simplex in R^n . Then T_1 is just a line segment, T_2 is a triangle, and T_3 is a tetrahedron with four vertices. The exact definition can be found in Fleming [3].

Let v_i , $1 \leq i \leq n+1$ be the vertices of T_n . Then any point $x \in T_n$ can be written as a convex combination of the vertices:

$$x = \sum_{i=1}^{n+1} c_i v_i, \quad \sum_{i=1}^{n+1} c_i = 1, \quad c_i \geq 0.$$

The numbers c_1, \dots, c_{n+1} are called the barycentric coordinates of x .

For any n -simplex T_n , the evenly spaced points of degree l are those points whose barycentric coordinates are of the form

$$(\frac{k_1}{l}, \frac{k_2}{l}, \dots, \frac{k_{n+1}}{l}), \quad k_i \text{ nonnegative integers with } \sum_{i=1}^{n+1} k_i = l.$$

Obviously, the number of evenly spaced points of degree l is $N = \binom{n+l}{n}$. It's proven in Bos [4] that such points do form a determining set for P_l^n .

Before entering our core theorem, some ingredients must be explained. Each function of the form (1) induces a function space $\mathcal{C}_{h,m}$, $m = \max\{0, \lceil \frac{\beta}{2} \rceil\}$, called native space. Also, there is a seminorm $\|f\|_h$ for each $f \in \mathcal{C}_{h,m}$. These can be found in Luh [5, 6, 7], Madych and Nelson [1, 8] and Wendland [2]. The constants ρ and Δ_0 , which are usually very small positive numbers for low dimensions, in the theorem are determined by n and β . We omit their complicated definitions and refer the reader to Luh [9].

The following theorem is just our core theorem. We omit its complicated proof and take it directly from [9].

Theorem 1.2 *Let h be as in (1). For any positive number b_0 , let $C = \max\left\{\frac{2}{3b_0}, \frac{8\rho}{c}\right\}$ and $\delta_0 = \frac{1}{3C}$. For any n -simplex T_n of diameter r satisfying $\frac{1}{3C} \leq r \leq \frac{2}{3C}$ (note that $\frac{2}{3C} \leq b_0$), if $f \in \mathcal{C}_{h,m}$,*

$$|f(x) - s(x)| \leq 2^{\frac{n+\beta-7}{4}} \pi^{\frac{n-1}{4}} \sqrt{n\alpha_n} c^{\frac{\beta}{2}} \sqrt{\Delta_0} \sqrt{3C} \sqrt{\delta} (\lambda')^{\frac{1}{\delta}} \|f\|_h \quad (3)$$

holds for all $x \in T_n$ and $0 < \delta \leq \delta_0$, where $s(x)$ is defined as in (2) with x_1, \dots, x_N the evenly spaced points of degree l in T_n satisfying $\frac{1}{3C\delta} \leq l \leq \frac{2}{3C\delta}$. The constant α_n denotes the volume of the unit

ball in R^n , and $0 < \lambda' < 1$ is given by

$$\lambda' = \left(\frac{2}{3}\right)^{\frac{1}{3C}}$$

which only in some cases mildly depends on the dimension n .

Remark. Note that as the degree l of the evenly spaced data points increases, the number δ will decrease, making the upper bound in (3) small. Hence δ can be regarded in spirit as the well-known fill distance. It is natural to ask what will happen if one regards δ completely the same as the fill distance. If so, the requirement that the centers x_1, \dots, x_N be evenly spaced in the simplex can be dropped, making this theorem much more useful. In fact, this is just the central idea of this paper.

2 Criteria of choosing c

The number b_0 in Theorem 1.2 controls the diameter of the domain. The upper bound in (3) is greatly related to the choice of c . In Luh [9] (3) is successfully transformed into a pleasant and lucid form which shows the influence of c explicitly. There are three cases: (i) $\beta > 0$ and $n \geq 1$, (ii) $\beta < 0$ and $n + \beta \geq 1$, or $n + \beta = -1$, and (iii) $\beta = -1$ and $n = 1$.

For (i) and (ii), we have

$$|f(x) - s(x)| \leq d_0 \sigma^{\frac{1+\beta+n}{4}} MN(c) \|f\|_{L^2(R^n)} \quad (4)$$

where d_0 is a small (for low dimensions) constant independent of c , σ , and f , and $MN(c)$ is a function of c defined by

$$MN(c) := \begin{cases} \sqrt{8\rho} \cdot c^{\frac{\beta-1-n}{4}} \cdot e^{\frac{c\sigma}{2}} \cdot \left(\frac{2}{3}\right)^{\frac{c}{24\delta\rho}} & \text{if } 24\rho\delta \leq c < 12\rho b_0, \\ \sqrt{\frac{2}{3b_0}} \cdot c^{\frac{1+\beta-n}{4}} \cdot e^{\frac{c\sigma}{2}} \cdot \left(\frac{2}{3}\right)^{\frac{b_0}{2\delta}} & \text{if } c \geq 12\rho b_0. \end{cases} \quad (5)$$

For (iii), we have

$$|f(x) - s(x)| \leq d'_0 MN(c) \|f\|_{L^2(R^n)}, \quad (6)$$

where d'_0 is only a bit different from d_0 , and $MN(c)$ is defined by

$$MN(c) := \begin{cases} \sqrt{8\rho} \cdot c^{\frac{\beta-1}{2}} \cdot \left(\frac{2}{3}\right)^{\frac{c}{24\delta\rho}} M(c) & \text{if } 24\rho\delta \leq c < 12\rho b_0, \\ \sqrt{\frac{2}{3b_0}} \cdot c^{\frac{\beta}{2}} \cdot \left(\frac{2}{3}\right)^{\frac{b_0}{2\delta}} M(c) & \text{if } c \geq 12\rho b_0, \end{cases} \quad (7)$$

where $M(c)$ is defined by

$$M(c) := \begin{cases} \frac{1}{\sqrt{\mathcal{K}_0(1)}} & \text{if } c \leq \frac{1}{\sigma}, \\ \left\{ \frac{1}{\mathcal{K}_0(1)} + 2\sqrt{3}\sqrt{c\sigma}e^{c\sigma} \right\}^{1/2} & \text{if } c > \frac{1}{\sigma}, \end{cases}$$

\mathcal{K}_0 being the modified Bessel function, for $c \in [24\rho\delta, \infty)$.

In the following text of this section the interpolation domain is a simplex in R^n and the parameter δ is interpreted as the well-known fill distance. For the definition of fill distance, we refer the

reader to Madych and Nelson [8] and Wendland [2]. Then we have the following criteria of choosing c .

Case 1. Let $f \in B_\sigma$, $\sigma > 0$. If (i) or (ii) holds, for any given $b_0 > 0$ and $\delta < \frac{b_0}{2}$, the optimal choice of c in the interval $[24\rho\delta, \infty)$ for the interpolation of f by s defined in (2) in a simplex of diameter less than or equal to b_0 is the number minimizing $MN(c)$ in (5).

Case 2. Let $f \in B_\sigma$, $\sigma > 0$. If (iii) holds, for any given $b_0 > 0$ and $\delta < \frac{b_0}{2}$, the optimal choice of c in the interval $[24\rho\delta, \infty)$ for the interpolation of f by s defined in (2) in a simplex of diameter less than or equal to b_0 is the number minimizing $MN(c)$ in (7).

The number ρ in this paper is always equal or close to 1 and $24\rho\delta$ is usually very small. Furthermore, experiments show that the optimal value of c never falls into the interval $(0, 24\rho\delta)$. Hence we have essentially dealt with $c \in (0, \infty)$. The relaxation of δ from its original definition to fill distance is natural and reasonable since in Theorem 1.2 it behaves in spirit exactly the same as the fill distance. As for the shape of the domain, we do not know how important it is. Maybe more experimental evidences should be collected first. For now, it does not seem to be possible to get rid of the simplex requirement in Theorem 1.2, both in theory and practice.

3 Experiments

We provide two sets of experiments here. Although we concern ourselves mainly with the scattered data setting, as a comparison, the evenly spaced data setting is also tested.

3.1 The evenly spaced data setting

Let us investigate Case 2. of the last section, i.e., $\beta = -1$ and $n = 1$. Suppose $\sigma = 1, b_0 = 5$. The curves of the MN function $MN(c)$ are presented in Figures 1-5, where δ was defined in Theorem 1.2.

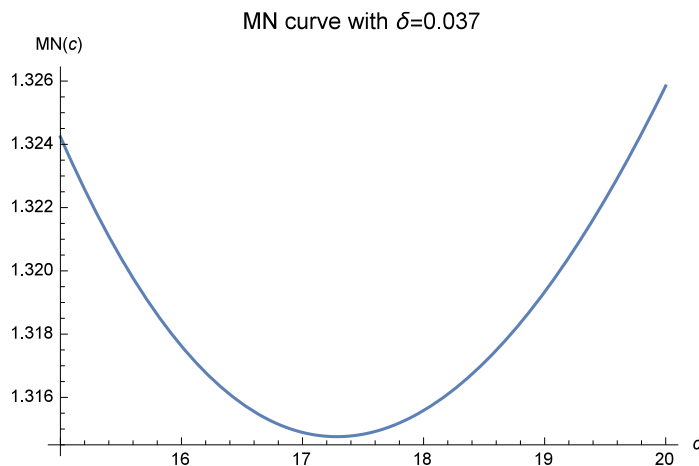


Figure 1: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

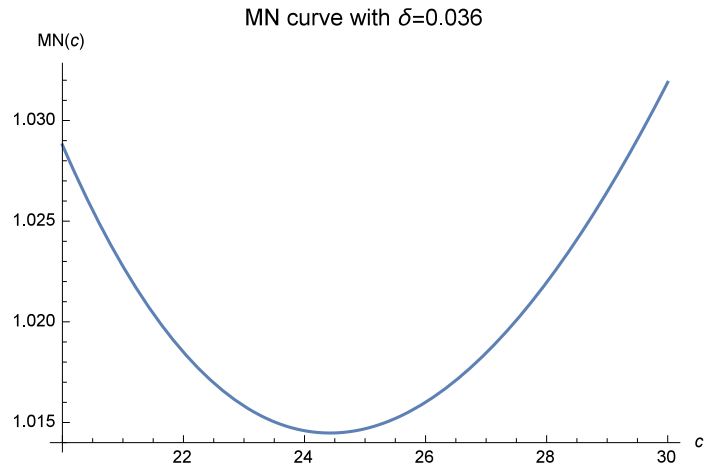


Figure 2: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

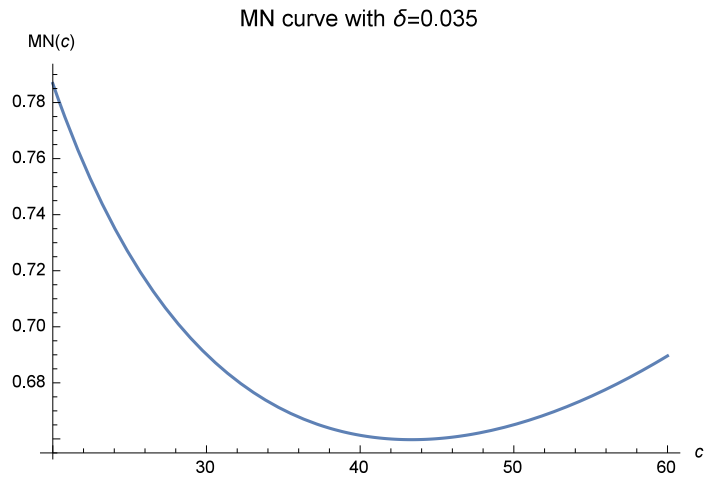


Figure 3: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

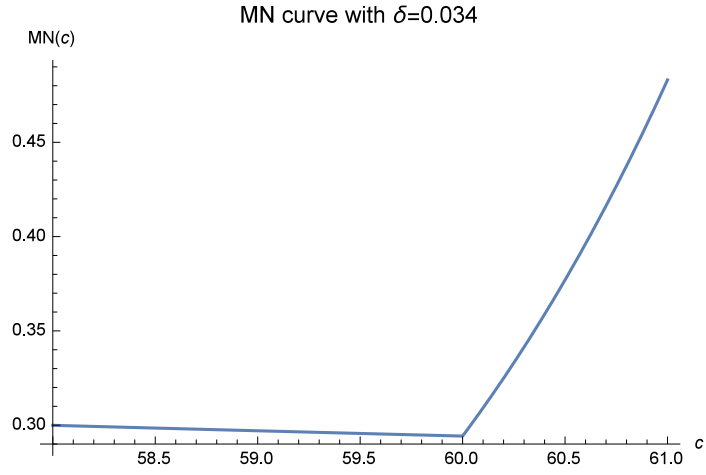


Figure 4: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

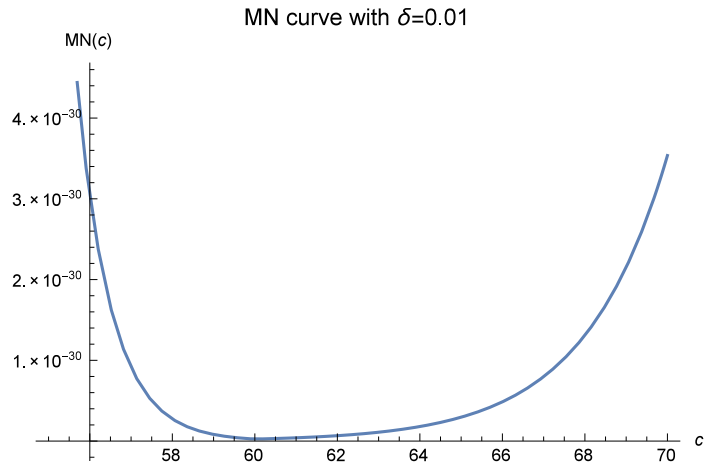


Figure 5: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

In Figures 1-5, one easily finds that as δ decreases, the optimal values of c move rapidly to 60. It strongly suggests that one should choose $c = 60$ as the optimal value. Now we can start our experiment.

In this experiment the approximated function adopted is

$$f(x) := \begin{cases} \frac{\sin x}{x} & \text{if } x \neq 0 \\ 1 & \text{if } x = 0. \end{cases}$$

It is easy to check that $f \in B_\sigma$ for $\sigma = 1$. We use $s(x)$ defined in (2) to interpolate $f(x)$ in the interval $[0, 5]$. However, for simplicity, the radial function used is the one mentioned in the abstract, rather than that of (1). The numbers of the centers (interpolation points) and test points are denoted by N_d and N_t , respectively. The centers x_1, \dots, x_{N_d} are evenly spaced in $[0, 5]$, and so are the test points z_1, \dots, z_{N_t} . We use the root-mean-square error RMS to evaluate the closeness of the approximation and define

$$RMS := \sqrt{\frac{\sum_{j=1}^{N_t} |f(z_j) - s(z_j)|^2}{N_t}}.$$

The condition number of the interpolation matrix is denoted by $COND$. As is well known, the condition numbers in the RBF interpolation are usually very large. The problem of ill-conditioning is overcome by adopting enough effective digits to the right of the decimal point, with the help of the arbitrarily precise computer software Mathematica. For example, if the condition number is 10^{150} , we adopt at least 200 effective digits for each step of the computation. Whenever keeping 250, 300, or even more effective digits, the final results are exactly the same, it means that the ill-conditioning has been completely controlled. Therefore our results should be reliable.

There is a logical problem in our approach. According to Theorem 2.1, one should choose c before determining the other parameters. However, we do not know in advance the optimal choice of c . Hence we fix b_0, σ, n, β , and δ first. Then the optimal c can be predicted by the curves of the $MN(c)$. Once c is chosen, we begin to arrange the centers according to Theorem 2.1. Here we let $l = \lfloor \frac{2}{3C\delta} \rfloor$. The results are presented in Tables 1-7.

Table 1: $\delta = 0.44$

c	20	30	40	50	60	70
RMS	$1.5 \cdot 10^{-2}$	$6.4 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$4.0 \cdot 10^{-7}$	$6.4 \cdot 10^{-9}$	$7.2 \cdot 10^{-9}$
$COND$	$2.1 \cdot 10^6$	$4.2 \cdot 10^{12}$	$4.3 \cdot 10^{19}$	$1.4 \cdot 10^{27}$	$1.1 \cdot 10^{35}$	$3.2 \cdot 10^{36}$
N_d	4	6	8	10	12	12
N_t	50	50	50	50	50	50
c	80	90	100			
RMS	$7.7 \cdot 10^{-9}$	$8.1 \cdot 10^{-9}$	$8.4 \cdot 10^{-9}$			
$COND$	$6.0 \cdot 10^{37}$	$7.9 \cdot 10^{38}$	$8.1 \cdot 10^{39}$			
N_d	12	12	12			
N_t	50	50	50			

Table 2: $\delta = 0.4$

c	20	30	40	50	60	70
RMS	$4.2 \cdot 10^{-3}$	$1.3 \cdot 10^{-4}$	$3.0 \cdot 10^{-6}$	$5.2 \cdot 10^{-8}$	$6.9 \cdot 10^{-10}$	$8.1 \cdot 10^{-10}$
$COND$	$4.3 \cdot 10^8$	$1.9 \cdot 10^{15}$	$3.4 \cdot 10^{22}$	$1.7 \cdot 10^{30}$	$1.9 \cdot 10^{38}$	$7.7 \cdot 10^{39}$
N_d	5	7	9	11	13	13
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$9.0 \cdot 10^{-10}$	$9.6 \cdot 10^{-10}$	$1.0 \cdot 10^{-9}$			
$COND$	$1.9 \cdot 10^{41}$	$3.2 \cdot 10^{42}$	$4.0 \cdot 10^{43}$			
N_d	13	13	13			
N_t	150	150	150			

Table 3: $\delta = 0.36$

c	20	30	40	50	60	70
RMS	$4.2 \cdot 10^{-3}$	$1.3 \cdot 10^{-4}$	$3.3 \cdot 10^{-7}$	$5.3 \cdot 10^{-9}$	$6.6 \cdot 10^{-11}$	$8.0 \cdot 10^{-11}$
$COND$	$4.3 \cdot 10^8$	$1.9 \cdot 10^{15}$	$2.5 \cdot 10^{25}$	$2.0 \cdot 10^{33}$	$3.2 \cdot 10^{41}$	$1.7 \cdot 10^{43}$
N_d	5	7	10	12	14	14
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$9.0 \cdot 10^{-11}$	$9.7 \cdot 10^{-11}$	$1.0 \cdot 10^{-10}$			
$COND$	$5.6 \cdot 10^{44}$	$1.2 \cdot 10^{46}$	$1.8 \cdot 10^{47}$			
N_d	14	14	14			
N_t	150	150	150			

Table 4: $\delta = 0.32$

c	20	30	40	50	60	70
RMS	$5.1 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$	$3.8 \cdot 10^{-8}$	$4.6 \cdot 10^{-11}$	$4.7 \cdot 10^{-13}$	$6.5 \cdot 10^{-13}$
$COND$	$7.6 \cdot 10^{10}$	$7.7 \cdot 10^{17}$	$2.0 \cdot 10^{28}$	$2.8 \cdot 10^{39}$	$9.4 \cdot 10^{47}$	$9.6 \cdot 10^{49}$
N_d	6	8	11	14	16	16
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$7.8 \cdot 10^{-13}$	$8.9 \cdot 10^{-13}$	$9.6 \cdot 10^{-13}$			
$COND$	$5.2 \cdot 10^{51}$	$1.8 \cdot 10^{53}$	$4.2 \cdot 10^{54}$			
N_d	16	16	16			
N_t	150	150	150			

Table 5: $\delta = 0.28$

c	20	30	40	50	60	70
RMS	$5.1 \cdot 10^{-4}$	$2.0 \cdot 10^{-6}$	$3.5 \cdot 10^{-9}$	$3.4 \cdot 10^{-12}$	$2.3 \cdot 10^{-15}$	$3.8 \cdot 10^{-15}$
$COND$	$7.6 \cdot 10^{10}$	$3.5 \cdot 10^{20}$	$1.5 \cdot 10^{31}$	$3.4 \cdot 10^{42}$	$2.8 \cdot 10^{54}$	$5.3 \cdot 10^{56}$
N_d	3	9	12	15	18	18
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$5.1 \cdot 10^{-15}$	$6.2 \cdot 10^{-15}$	$2.2 \cdot 10^{-13}$			
$COND$	$4.9 \cdot 10^{58}$	$2.7 \cdot 10^{60}$	$6.7 \cdot 10^{62}$			
N_d	18	18	18			
N_t	150	150	150			

Table 6: $\delta = 0.24$

c	20	30	40	50	60	70
RMS	$7.7 \cdot 10^{-5}$	$1.5 \cdot 10^{-8}$	$2.0 \cdot 10^{-11}$	$6.9 \cdot 10^{-16}$	$2.6 \cdot 10^{-19}$	$8.4 \cdot 10^{-19}$
$COND$	$1.5 \cdot 10^{13}$	$6.4 \cdot 10^{25}$	$8.6 \cdot 10^{36}$	$5.7 \cdot 10^{51}$	$1.5 \cdot 10^{64}$	$7.0 \cdot 10^{66}$
N_d	3	11	14	18	21	21
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$1.5 \cdot 10^{-18}$	$2.1 \cdot 10^{-18}$	$2.6 \cdot 10^{-18}$			
$COND$	$1.4 \cdot 10^{69}$	$1.6 \cdot 10^{71}$	$1.1 \cdot 10^{73}$			
N_d	21	21	21			
N_t	150	150	150			

Table 7: $\delta = 0.20$

c	20	30	40	50	60	70
RMS	$2.0 \cdot 10^{-7}$	$9.3 \cdot 10^{-12}$	$1.5 \cdot 10^{-15}$	$5.2 \cdot 10^{-20}$	$7.0 \cdot 10^{-25}$	$2.3 \cdot 10^{-24}$
$COND$	$5.6 \cdot 10^{17}$	$1.2 \cdot 10^{31}$	$4.0 \cdot 10^{45}$	$1.0 \cdot 10^{61}$	$1.3 \cdot 10^{77}$	$2.1 \cdot 10^{80}$
N_d	9	13	17	21	25	25
N_t	150	150	150	150	150	150
c	80	90	100			
RMS	$1.0 \cdot 10^{-23}$	$2.2 \cdot 10^{-23}$	$3.3 \cdot 10^{-23}$			
$COND$	$1.3 \cdot 10^{83}$	$3.6 \cdot 10^{85}$	$5.7 \cdot 10^{87}$			
N_d	25	25	25			
N_t	150	150	150			

In Tables 1-7 it is easily seen that the optimal values of c are always 60, as predicted by the MN curves. Hence our approach of finding the optimal c is extremely reliable for the evenly spaced data setting. What is noteworthy is that in these tables, the numbers of data points used are not always the same, for the same δ . This results from the requirement of Theorem 1.2. According to Theorem 1.2, one should choose c first and then arrange the centers by the value of c .

3.2 The scattered data setting

Now we begin to test our theoretical prediction of the optimal value of c when the data points are purely scattered. We use the Mathematica command `Random[.]` to generate a random number between 0 and 1. The interpolation domain is still $[0, 5]$. The interval $[0, 5]$ is divided into subintervals of width δ . Each subinterval contains a random number. For example, if $[a_i, b_i]$ is a subinterval, then $x_i = a_i + \text{Random}[.] * \delta$ is an interpolation center in this subinterval. If $5/\delta$ is not an integer, then 5 is set to be the interpolation center of the rightmost subinterval. Obviously the fill distance in this setting is δ . Then we use $s(x)$ in (2) with the gamma function replaced by 1 to interpolate $f(x)$ defined in subsection 3.1. The results are presented in Tables 8-14.

Table 8: $\delta = 0.48$

c	10	16	18	20	30	40
RMS	$1.4 \cdot 10^{-7}$	$1.4 \cdot 10^{-8}$	$1.2 \cdot 10^{-8}$	$2.1 \cdot 10^{-8}$	$3.8 \cdot 10^{-8}$	$1.0 \cdot 10^{-7}$
$COND$	$1.2 \cdot 10^{17}$	$1.1 \cdot 10^{21}$	$1.1 \cdot 10^{22}$	$8.6 \cdot 10^{22}$	$2.7 \cdot 10^{26}$	$8.2 \cdot 10^{28}$
N_d	11	11	11	11	11	11
N_t	40	40	40	40	40	40
c	50	60	70			
RMS	$1.4 \cdot 10^{-7}$	$6.8 \cdot 10^{-8}$	$7.5 \cdot 10^{-8}$			
$COND$	$7.1 \cdot 10^{30}$	$1.5 \cdot 10^{32}$	$3.3 \cdot 10^{33}$			
N_d	11	11	11			
N_t	40	40	40			

Table 9: $\delta = 0.40$

c	20	25	28	30	40	50
RMS	$1.6 \cdot 10^{-10}$	$1.4 \cdot 10^{-10}$	$1.1 \cdot 10^{-10}$	$3.4 \cdot 10^{-11}$	$5.9 \cdot 10^{-10}$	$1.2 \cdot 10^{-9}$
$COND$	$7.8 \cdot 10^{27}$	$1.6 \cdot 10^{30}$	$2.4 \cdot 10^{31}$	$1.2 \cdot 10^{32}$	$1.2 \cdot 10^{35}$	$2.5 \cdot 10^{37}$
N_d	13	13	13	13	13	13
N_t	80	80	80	80	80	80
c	60	70	90	120		
RMS	$1.6 \cdot 10^{-9}$	$1.8 \cdot 10^{-9}$	$2.2 \cdot 10^{-9}$	$2.4 \cdot 10^{-9}$		
$COND$	$2.0 \cdot 10^{39}$	$7.9 \cdot 10^{40}$	$3.3 \cdot 10^{43}$	$3.3 \cdot 10^{46}$		
N_d	13	13	13	13		
N_t	80	80	80	80		

Table 10: $\delta = 0.32$

c	20	25	30	40	50	60
RMS	$4.4 \cdot 10^{-13}$	$2.8 \cdot 10^{-13}$	$1.0 \cdot 10^{-13}$	$1.3 \cdot 10^{-13}$	$1.1 \cdot 10^{-12}$	$2.0 \cdot 10^{-12}$
$COND$	$5.8 \cdot 10^{34}$	$4.4 \cdot 10^{37}$	$1.0 \cdot 10^{40}$	$5.5 \cdot 10^{43}$	$4.4 \cdot 10^{46}$	$1.0 \cdot 10^{49}$
N_d	16	16	16	16	16	16
N_t	80	80	80	80	80	80
c	70	90	120			
RMS	$2.7 \cdot 10^{-12}$	$3.7 \cdot 10^{-12}$	$4.5 \cdot 10^{-12}$			
$COND$	$1.1 \cdot 10^{51}$	$2.0 \cdot 10^{54}$	$1.1 \cdot 10^{58}$			
N_d	16	16	16			
N_t	80	80	80			

Table 11: $\delta = 0.24$

c	20	30	40	48	50	52
RMS	$7.5 \cdot 10^{-18}$	$2.7 \cdot 10^{-19}$	$7.3 \cdot 10^{-20}$	$1.2 \cdot 10^{-19}$	$1.0 \cdot 10^{-19}$	$4.8 \cdot 10^{-20}$
$COND$	$9.7 \cdot 10^{45}$	$9.6 \cdot 10^{52}$	$9.2 \cdot 10^{57}$	$1.3 \cdot 10^{61}$	$6.8 \cdot 10^{61}$	$3.2 \cdot 10^{62}$
N_d	21	21	21	21	21	21
N_t	80	80	80	80	80	80
c	54	56	60	70		
RMS	$4.2 \cdot 10^{-20}$	$1.6 \cdot 10^{-19}$	$4.9 \cdot 10^{-19}$	$1.6 \cdot 10^{-18}$		
$COND$	$1.5 \cdot 10^{63}$	$6.3 \cdot 10^{63}$	$9.9 \cdot 10^{64}$	$4.7 \cdot 10^{67}$		
N_d	21	21	21	21		
N_t	80	80	80	80		

Table 12: $\delta = 0.20$

c	20	30	40	48	50	52
RMS	$5.0 \cdot 10^{-21}$	$5.1 \cdot 10^{-24}$	$8.8 \cdot 10^{-24}$	$5.0 \cdot 10^{-24}$	$4.1 \cdot 10^{-24}$	$1.5 \cdot 10^{-24}$
$COND$	$3.3 \cdot 10^{55}$	$8.1 \cdot 10^{63}$	$7.7 \cdot 10^{69}$	$4.8 \cdot 10^{73}$	$3.4 \cdot 10^{74}$	$2.2 \cdot 10^{75}$
N_d	25	25	25	25	25	25
N_t	80	80	80	80	80	80
c	54	56	60	70		
RMS	$1.8 \cdot 10^{-24}$	$4.7 \cdot 10^{-24}$	$7.1 \cdot 10^{-24}$	$2.4 \cdot 10^{-23}$		
$COND$	$1.4 \cdot 10^{76}$	$7.7 \cdot 10^{76}$	$2.1 \cdot 10^{78}$	$3.4 \cdot 10^{81}$		
N_d	25	25	25	25		
N_t	80	80	80	80		

Table 13: $\delta = 0.17$

c	20	30	40	50	54	56
RMS	$1.0 \cdot 10^{-26}$	$1.4 \cdot 10^{-29}$	$1.2 \cdot 10^{-30}$	$1.6 \cdot 10^{-31}$	$2.0 \cdot 10^{-31}$	$6.5 \cdot 10^{-32}$
$COND$	$1.2 \cdot 10^{66}$	$1.7 \cdot 10^{76}$	$2.8 \cdot 10^{83}$	$1.1 \cdot 10^{89}$	$9.9 \cdot 10^{90}$	$8.1 \cdot 10^{91}$
N_d	30	30	30	30	30	30
N_t	80	80	80	80	80	80
c	58	60	70	100	120	
RMS	$7.9 \cdot 10^{-32}$	$1.8 \cdot 10^{-31}$	$2.4 \cdot 10^{-31}$	$1.1 \cdot 10^{-29}$	$3.2 \cdot 10^{-29}$	
$COND$	$6.2 \cdot 10^{92}$	$4.4 \cdot 10^{93}$	$3.3 \cdot 10^{97}$	$3.2 \cdot 10^{106}$	$1.2 \cdot 10^{111}$	
N_d	30	30	30	30	30	
N_t	80	80	80	80	80	

Table 14: $\delta = 0.165$

c	40	50	55	60	65	70
RMS	$3.4 \cdot 10^{-31}$	$4.2 \cdot 10^{-32}$	$3.7 \cdot 10^{-32}$	$5.9 \cdot 10^{-34}$	$3.2 \cdot 10^{-32}$	$1.8 \cdot 10^{-33}$
$COND$	$2.0 \cdot 10^{87}$	$1.3 \cdot 10^{93}$	$3.9 \cdot 10^{95}$	$7.1 \cdot 10^{97}$	$8.7 \cdot 10^{99}$	$7.4 \cdot 10^{101}$
N_d	31	31	31	31	31	31
N_t	160	160	160	160	160	160
c	80	100	120			
RMS	$5.0 \cdot 10^{-32}$	$1.6 \cdot 10^{-30}$	$5.6 \cdot 10^{-30}$			
$COND$	$2.2 \cdot 10^{105}$	$1.4 \cdot 10^{111}$	$8.0 \cdot 10^{115}$			
N_d	31	31	31			
N_t	160	160	160			

As predicted by Figures 1-5, the optimal values of c will move to 60 when δ decreases. This is supported by the results in Tables 8-14, where δ is interpreted as the fill distance.

4 The failures of the MN curve approach

As is well known, Newton's method of root-finding may fail whenever there are horizontal or nearly horizontal tangent lines. Similarly, our approach may also fail whenever there are nearly horizontal zones on the MN curves. Let us see a few MN curves first. If we further decrease the parameter δ in Figures 1-5 of Section 3, nearly horizontal zones will appear, near the bottoms of the MN curves, as shown in Figures 6-8. Also, note that, for the same δ , the root-mean-square errors in the tables of the preceding section are much smaller than the error bounds (4) and (6) essentially reflected by the MN function values, shown in Figures 1-5. It means that the error bounds are not very sharp. Once the curve is nearly horizontal at the bottom, the optimal value of c predicted by the MN curve may not be reliable. The actual optimal value may fall into the nearly horizontal zone. The longer this zone is, the less reliable the MN curve approach is. Experiments also show this, both in the evenly spaced and scattered data settings. Our experimental results are presented in Tables 15-18 and 19-22 for the two settings, respectively, where the δ 's are smaller than those of Tables 7 and 14.

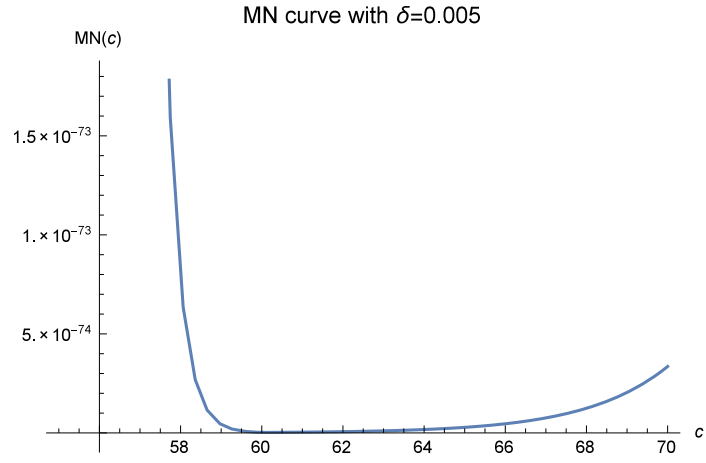


Figure 6: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

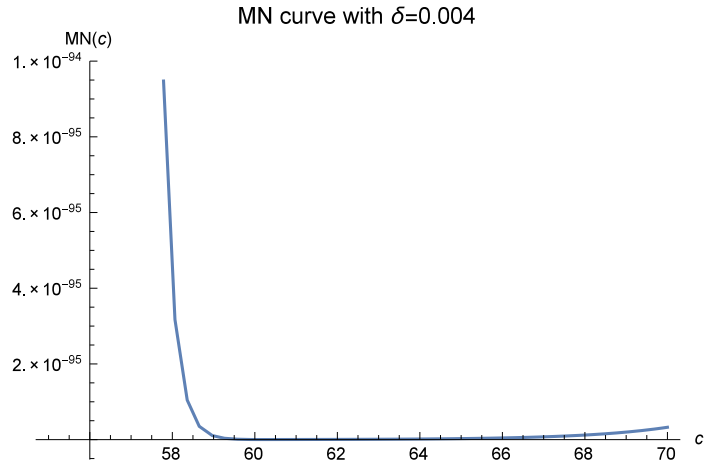


Figure 7: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

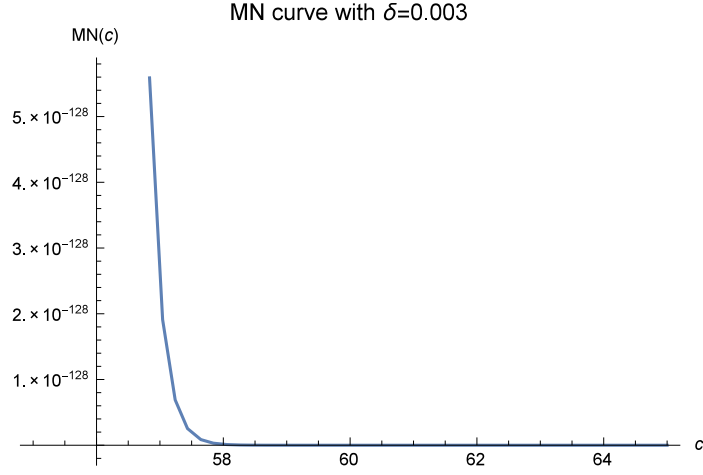


Figure 8: Here $n = 1$, $\beta = -1$, $b_0 = 5$ and $\sigma = 1$.

Table 15: $\delta = 0.16$

c	40	50	60	70	80	90
RMS	$3.8 \cdot 10^{-20}$	$3.1 \cdot 10^{-28}$	$1.9 \cdot 10^{-34}$	$1.7 \cdot 10^{-34}$	$5.4 \cdot 10^{-34}$	$1.8 \cdot 10^{-33}$
$COND$	$1.4 \cdot 10^{57}$	$3.0 \cdot 10^{79}$	$5.8 \cdot 10^{99}$	$8.2 \cdot 10^{103}$	$3.2 \cdot 10^{107}$	$4.7 \cdot 10^{110}$
N_d	21	27	32	32	32	32
N_t	119	119	119	119	119	119
c	100	110	120			
RMS	$1.0 \cdot 10^{-32}$	$2.4 \cdot 10^{-32}$	$4.2 \cdot 10^{-32}$			
$COND$	$3.2 \cdot 10^{113}$	$1.2 \cdot 10^{116}$	$2.6 \cdot 10^{118}$			
N_d	32	32	32			
N_t	119	119	119			

Table 16: $\delta = 0.12$

c	30	40	50	60	70	80
RMS	$1.4 \cdot 10^{-19}$	$2.8 \cdot 10^{-28}$	$7.4 \cdot 10^{-38}$	$8.1 \cdot 10^{-48}$	$1.1 \cdot 10^{-48}$	$4.8 \cdot 10^{-50}$
$COND$	$1.4 \cdot 10^{52}$	$2.1 \cdot 10^{77}$	$1.3 \cdot 10^{104}$	$1.4 \cdot 10^{132}$	$4.2 \cdot 10^{137}$	$2.4 \cdot 10^{142}$
N_d	21	28	35	42	42	42
N_t	150	150	150	150	150	150
c	90	100	110			
RMS	$2.0 \cdot 10^{-49}$	$2.7 \cdot 10^{-49}$	$4.5 \cdot 10^{-48}$			
$COND$	$3.7 \cdot 10^{146}$	$2.1 \cdot 10^{150}$	$5.1 \cdot 10^{153}$			
N_d	42	42	42			
N_t	150	150	150			

Table 17: $\delta = 0.08$

c	60	70	80	90	100	110
RMS	$3.8 \cdot 10^{-76}$	$2.1 \cdot 10^{-78}$	$4.8 \cdot 10^{-80}$	$9.4 \cdot 10^{-81}$	$1.2 \cdot 10^{-81}$	$1.6 \cdot 10^{-82}$
$COND$	$1.3 \cdot 10^{200}$	$2.6 \cdot 10^{208}$	$4.0 \cdot 10^{215}$	$8.7 \cdot 10^{221}$	$4.1 \cdot 10^{227}$	$5.5 \cdot 10^{232}$
N_d	63	63	63	63	63	63
N_t	150	150	150	150	150	150
c	120	130	150			
RMS	$2.9 \cdot 10^{-82}$	$3.4 \cdot 10^{-82}$	$4.7 \cdot 10^{-82}$			
$COND$	$2.7 \cdot 10^{237}$	$5.4 \cdot 10^{241}$	$2.8 \cdot 10^{249}$			
N_d	63	63	63			
N_t	150	150	150			

Table 18: $\delta = 0.06$

c	80	90	100	110	120	140
RMS	$3.4 \cdot 10^{-110}$	$3.3 \cdot 10^{-112}$	$5.4 \cdot 10^{-114}$	$1.2 \cdot 10^{-115}$	$3.1 \cdot 10^{-116}$	$6.2 \cdot 10^{-118}$
$COND$	$6.6 \cdot 10^{288}$	$2.0 \cdot 10^{297}$	$7.9 \cdot 10^{304}$	$5.9 \cdot 10^{311}$	$1.1 \cdot 10^{318}$	$1.4 \cdot 10^{329}$
N_d	84	84	84	84	84	84
N_t	329	329	329	329	329	329
c	160	170	180	200		
RMS	$4.9 \cdot 10^{-118}$	$4.4 \cdot 10^{-118}$	$5.3 \cdot 10^{-118}$	$1.6 \cdot 10^{-117}$		
$COND$	$6.0 \cdot 10^{338}$	$1.4 \cdot 10^{343}$	$1.8 \cdot 10^{347}$	$7.2 \cdot 10^{354}$		
N_d	84	84	84	84		
N_t	329	329	329	329		

Table 19: $\delta = 0.12$

c	50	60	70	80	90	100
RMS	$1.7 \cdot 10^{-46}$	$3.1 \cdot 10^{-47}$	$3.9 \cdot 10^{-48}$	$2.5 \cdot 10^{-49}$	$8.6 \cdot 10^{-49}$	$5.0 \cdot 10^{-49}$
$COND$	$3.9 \cdot 10^{126}$	$1.2 \cdot 10^{133}$	$3.6 \cdot 10^{138}$	$2.1 \cdot 10^{143}$	$3.2 \cdot 10^{147}$	$1.6 \cdot 10^{151}$
N_d	42	42	42	42	42	42
N_t	160	160	160	160	160	160
c	110	120	130			
RMS	$9.4 \cdot 10^{-48}$	$3.9 \cdot 10^{-47}$	$2.4 \cdot 10^{-46}$			
$COND$	$4.0 \cdot 10^{154}$	$5.1 \cdot 10^{157}$	$3.6 \cdot 10^{160}$			
N_d	42	42	42			
N_t	160	160	160			

Table 20: $\delta = 0.08$

c	50	60	70	80	90	100
RMS	$3.0 \cdot 10^{-72}$	$8.8 \cdot 10^{-76}$	$4.5 \cdot 10^{-78}$	$1.3 \cdot 10^{-76}$	$2.2 \cdot 10^{-80}$	$2.9 \cdot 10^{-81}$
$COND$	$3.2 \cdot 10^{191}$	$2.6 \cdot 10^{201}$	$5.1 \cdot 10^{209}$	$7.8 \cdot 10^{216}$	$1.7 \cdot 10^{223}$	$8.0 \cdot 10^{228}$
N_d	63	63	63	63	63	63
N_t	320	320	320	320	320	320
c	110	120	130	140		
RMS	$3.2 \cdot 10^{-82}$	$6.8 \cdot 10^{-82}$	$7.9 \cdot 10^{-82}$	$1.0 \cdot 10^{-81}$		
$COND$	$1.1 \cdot 10^{234}$	$5.2 \cdot 10^{238}$	$1.1 \cdot 10^{243}$	$1.0 \cdot 10^{247}$		
N_d	63	63	63	63		
N_t	320	320	320	320		

Table 21: $\delta = 0.06$

c	50	60	70	80	90	100
RMS	$1.1 \cdot 10^{-98}$	$3.6 \cdot 10^{-103}$	$9.1 \cdot 10^{-107}$	$2.0 \cdot 10^{-109}$	$1.9 \cdot 10^{-111}$	$3.3 \cdot 10^{-113}$
$COND$	$1.4 \cdot 10^{256}$	$1.8 \cdot 10^{269}$	$2.3 \cdot 10^{280}$	$9.8 \cdot 10^{289}$	$3.0 \cdot 10^{298}$	$1.2 \cdot 10^{306}$
N_d	84	84	84	84	84	84
N_t	320	320	320	320	320	320

c	110	120	130	140	150
RMS	$6.7 \cdot 10^{-115}$	$1.9 \cdot 10^{-115}$	$2.0 \cdot 10^{-116}$	$5.0 \cdot 10^{-113}$	$6.0 \cdot 10^{-107}$
$COND$	$8.7 \cdot 10^{312}$	$1.6 \cdot 10^{319}$	$9.5 \cdot 10^{324}$	$2.1 \cdot 10^{330}$	$2.0 \cdot 10^{335}$
N_d	84	84	84	84	84
N_t	320	320	320	320	320

Table 22: $\delta = 0.03$

c	40	60	80	100	120	140
RMS	$5.4 \cdot 10^{-189}$	$3.3 \cdot 10^{-213}$	$1.0 \cdot 10^{-229}$	$1.5 \cdot 10^{-241}$	$2.1 \cdot 10^{-250}$	$3.5 \cdot 10^{-257}$
$COND$	$3.4 \cdot 10^{479}$	$8.1 \cdot 10^{537}$	$2.3 \cdot 10^{579}$	$3.3 \cdot 10^{611}$	$6.3 \cdot 10^{637}$	$1.0 \cdot 10^{660}$
N_d	167	167	167	167	167	167
N_t	700	700	700	700	700	700
c	160	170	180	190	200	
RMS	$1.5 \cdot 10^{-262}$	$7.2 \cdot 10^{-265}$	$2.5 \cdot 10^{-269}$	$7.2 \cdot 10^{-266}$	$5.0 \cdot 10^{-259}$	
$COND$	$1.9 \cdot 10^{679}$	$1.0 \cdot 10^{688}$	$1.8 \cdot 10^{696}$	$1.1 \cdot 10^{704}$	$2.8 \cdot 10^{711}$	
N_d	167	167	167	167	167	
N_t	700	700	700	700	700	

It is easily seen that in Tables 15-18, the evenly spaced data setting, the optimal values of c go away from the theoretically predicted value 60 as the parameter δ decreases. It is the same for the scattered data setting, as shown in Tables 19-22. Therefore, one must be careful whenever the bottom of the MN curve tends to be horizontal.

5 Summary

We are satisfied with the performance of the MN curve approach to finding the optimal value of the shape parameter, both in the evenly spaced and purely scattered data settings. Although this approach was presented by the author, the foundation built by W.R. Madych and S.A. Nelson plays an important role. Based on this foundation, the author eventually presented a practically useful theory. Hence we name the crucial function MN function, in honor of their outstanding contribution. It is natural to ask whether our theory can be improved. To our regret, the answer probably is ‘no’. It is already known that algebraic-type error bounds do not reflect the influence of the shape parameter well. As for the exponential-type error bound raised by Madych and Nelson in [10], which applies to scattered data settings, shows the influence of the shape parameter sufficiently only when fill distance is extremely small, making it practically useless. This can be seen in Luh [11]. The improved exponential-type error bound, namely Theorem 1.2 of this paper, shows the influence of the shape parameter sufficiently when fill distance is of reasonable size. In the field of radial basis functions, this kind of exponential-type error bound probably is already optimal, due to the uncertainty principle subject to the condition number, as can be seen in Schaback [12]. It means that even if there is an exponential-type error bound which can be used to predict directly the optimal value of the shape parameter and applies to scattered data settings, it may not be better

than the approach developed from Theorem 1.2 of this paper.

As for the function space, although B_σ in Definition 1.1 is quite small, it plays only an intermediate role in the process of the interpolation. We repeatedly pointed out that any function in the Sobolev space, which contains the solutions to many important differential equations, can be interpolated by an B_σ function with a good error bound, as shown in Narcowich et al. [13]. Then the B_σ function can be interpolated by a function in the form of (2) with the same set of data points, also with a good error bound, of which the MN function $MN(c)$ is its essential part. The distance between the Sobolev space function and the RBF interpolator (2) can be handled by triangle inequality. The B_σ function need not be found explicitly. One only needs to know that it exists. The choice of the parameter σ is very flexible. As long as it makes both error bounds small, it is a good choice.

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